$\mathcal{PT}-$symmetric square well

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Abstract

Below a (comparatively large) measure of non-Hermiticity $Z = Z_0^{(crit)} > 0$ of a $\mathcal{PT}$ symmetrically complexified square well, bound states are constructed non-numerically. All their energies prove real and continuous in the (Hermitian) limit $Z \to 0$. Beyond the threshold $Z_0^{(crit)}$ (and, in general, beyond $Z_m^{(crit)}$ at $m = 0, 1, \ldots$) the lowest two real energies (i.e., E_{2m} and E_{2m+1}) are shown to merge and disappear.

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1 Introduction

An interest of physicists in complex potentials $V(x) = \mathrm{Re}\, V(x) + i\, \mathrm{Im}\, V(x)$ with the generalized symmetry property

$$\mathrm{Re}\, V(x) = \mathrm{Re}\, V(-x), \qquad \mathrm{Im}\, V(x) = -\mathrm{Im}\, V(-x) \tag{1}$$

dates back to the perturbative study of imaginary cubic anharmonic oscillators

$$V(x) = \omega\, x^2 + i\, \lambda\, x^3 \tag{2}$$

by Caliceti et al [1]. In the early nineties, an increase of this interest [2] was inspired by the role of the imaginary cubic anharmonicity in field theory where eq. (1) mimics the fundamental parity times time-reversal ($= \mathcal{PT}$) symmetry of phenomenological Lagrangians [3]. Under certain circumstances, the $\mathcal{PT}$ symmetric and Hermitian models can even prove mathematically equivalent [4].

In the late nineties, Bender and Boettcher [5] analysed the one-parametric family of the power-law $\omega \to 0$ models

$$V(x) = x^2\, (i\, x)^\delta \tag{3}$$

by the quasi-classical and purely numerical means. On this basis they conjectured that all the $\delta > 0$ bound-state energies $E_n = E_n(\delta)$ form a real and discrete, smooth continuation of the well known harmonic-oscillator $\delta = 0$ spectrum. An extension of this study inspired them later to apply the conjecture (formulated, originally, by Bessis at $\delta = 1$ [6]) to a still broader class of interactions. Within the resulting "generalized" (so called $\mathcal{PT}$ symmetric) quantum mechanics [7], there appears a growing number of interesting studies, promoting the ideas of supersymmetry [8, 9], exact semiclassical techniques [10], functional analysis [11] and perturbation theory [12]. All of them provide a consistent picture of a theory with certain (not quite well understood) limitations. Even in the above "guiding" example (3) the $\mathcal{PT}$ symmetry breaks down spontaneously at $\delta < 0$ [5].

Phenomenological appeal of the $\mathcal{PT}$ symmetric modifications need not even stop before the "sacred" quantum electrodynamics [13]. Still, the formalism abounds in open questions and its mathematical foundations are mostly conjectures. This is the reason why the attention quickly spreads from the phenomenologically oriented eq. (3) to its exactly solvable alternatives. In this direction, the partially solvable extension of the $\delta = 2$ quartic case [14] and the discovery of the exact solvability of the certain version of the $\delta \to \infty$ limiting case [8] were the first and encouraging successes. They were followed by the $\mathcal{PT}$ symmetric regularization of the more-dimensional harmonic oscillator [15] and by the formulation and solution of many further shape-invariant models [16]-[20].

Once we move beyond the domain of analytic potentials, numerical studies provide significantly less encouraging results [7]. This is the reason why the "most elementary" square well

$$\begin{array}{ll} \mathrm{Re}\, V(x) = 0, & x \in (-1,1) \\ \mathrm{Im}\, V(x) = Z, & x \in (-1,0) \\ \mathrm{Im}\, V(x) = -Z, & x \in (0,1) \end{array} \tag{4}$$

has always been $\mathcal{PT}$ symmetrized just in the (various, non-equivalent) $\delta \to \infty$ limits of eq. (3) [8, 21, 22].

2 Solution

Presumably, the reason for absence of the "forgotten" $\mathcal{PT}$ symmetric square well (4) in the literature lies in an ambiguity of its continuation beyond the discontinuities at $x = \pm 1$. We are going to treat this problem simply by imposing the Dirichlet boundary conditions on our (complex) wave functions,

$$\psi(\pm 1) = 0. \tag{5}$$

Having made the latter decision the explicit computations are really elementary. Their essence lies in the easy construction of the general right and left solutions

$$\begin{aligned} \psi_+ &= c_+ e^{\kappa\, x} + d_+ e^{-\kappa\, x} \\ \psi_- &= c_- e^{\kappa^*\, x} + d_- e^{-\kappa^*\, x} \end{aligned} \tag{6}$$

with the complex κ and its conjugate κ^*. We re-parametrize the (by assumption, real) energies $E = t^2 - s^2$ and the measure of non-Hermiticity $Z = 2st$. This gives the complex exponents $\kappa = s - it$ since $\kappa^2 = V(x) - E$ is also complex (and constant for all $x \in (0,1)$). Our solutions (6) are made explicit, for every real E and Z, when we use the inverse formulae

$$t = \frac{1}{\sqrt{2}} \left(E + \sqrt{E^2 + Z^2}\right)^{1/2},$$

$$s = \frac{Z}{\sqrt{2}} \left(E + \sqrt{E^2 + Z^2}\right)^{-1/2}.$$

In the light of the $\mathcal{PT}$ symmetry of our Hamiltonian $H = \mathcal{PT}H\mathcal{PT}$, the product $\mathcal{PT}\psi(x) \equiv \psi^*(-x)$ will satisfy the same Schrödinger equation as $\psi(x)$. Hence, in the origin, we are permitted to normalize our bound states in a $\mathcal{PT}$ symmetric way,

$$\psi_+(0) = \psi_-(0) = 1, \qquad \partial_x\psi_+(0) = \partial_x\psi_-(0) = i\,A.$$

These conditions contain a free real parameter A and are equivalent to the matching of wave functions,

$$c_\pm = 1 - d_\pm,$$

$$\kappa\,(1 - 2\,d_+) = \kappa^*(1 - 2\,d_-) = iA.$$

This implies that we know all the coefficients in eq. (6),

$$d_+ = \frac{1}{2} - i\,\frac{A}{2\kappa}, \qquad d_- = \frac{1}{2} - i\,\frac{A}{2\kappa^*}.$$

It is easy to satisfy the external boundary conditions (5) and reduce them to the elementary prescription

$$i\,A = -\kappa\,\coth\kappa. \tag{7}$$

In terms of the real parameters s and t this represents a system of two algebraic equations,

$$A = -\frac{s}{\tan t} + t\,\tanh s = s\,\tan t + \frac{t}{\tanh s}. \tag{8}$$

Its first part defines the (necessarily, real) value of $A = A(s,t)$. A re-arrangement of the second algebraic equation is elementary and gives the rule

$$-2t\,\sin 2t = 2s\,\sinh 2s. \tag{9}$$

As long as both its sides depend on the mere absolute values of the respective variables t and s, we may pick up $t \geq 0$, insert the definition of $s = Z/2t$ and solve this equation numerically.

3 Discussion

By construction, the spectrum of the real energies $E = E_n$ is defined in terms of the roots t_n of eq. (9), $E_n = t_n^2 - s_n^2$, $s_n = Z/2t_n$, $n = 0, 1, \ldots$. After we re-scale $t \to T = 2t/\pi$, we immediately see that in the limit $Z \to 0$ this spectrum degenerates to the known Hermitian one, with $T_n = n+1$ etc. From our equation (9) it is obvious that at the very small Z (and, hence, $s \approx 0$), the change of the above roots T_n (and, of course, energies) remains very small as well.

At the larger (and, say, positive) Z, the analysis of our quantization condition (9) becomes significantly simplified by the re-scalings $s \to S_0 = 2\,s\,\sinh 2s$ and $S_0 \to S$ such that, say, $S_0 = 4\,\sinh^2 S$. Both these steps represent a one-to-one mapping exhibiting the strict leading-order quasi-linearity $s \sim S$ achieved at both ends of our half-axis, i.e., for $s \approx 0$ as well as for $s \to \infty$. Moreover, this introduces just a minimal deformation of the scale of the coordinate s (practically invisible on a picture) and replaces equation (9) by a new one,

$$-\pi\,T\,\sin \pi T = 4\,\sinh^2 S. \tag{10}$$

This new relation is explicitly solvable. The resulting analytic and $Z-$independent formula $S = X(T)$ defines a curve in our new $S - T$ plane. Its $T < 14$ part is displayed in Figure 1.

In order to determine the separate roots T_n (and, hence, the spectrum of energies), it remains for us to recollect the $Z-$dependent, hyperbolic constraint $s = Z/2t$. After we translate its form in our new variables, $S = Y(Z,T)$, we discover that it has a monotonous, hyperbolic shape which depends on Z. Figure 1 offers a few samples. We may conclude that each point of the intersection of our two curves $X(T)$ and $Y(Z,T)$ determines a $Z-$dependent root $T = T(Z)$ and, hence, a real energy.

The $Z-$ dependence of the roots $T(Z)$ is, in general, smooth. A non-perturbative effect is only encountered at certain critical values $Z = Z^{(crit)}$. In the vicinity of these points, the two leftmost roots $T_0(Z) < T_1(Z)$, $Z < Z^{(crit)}$ merge in a single, doubly degenerate real root $T_0(Z^{(crit)}) = T_1(Z^{(crit)})$. Figure 1 gives two examples and shows that even the smallest one of these critical values is already quite large ($Z_0^{(crit)} \approx 4.48$). Below this bound we may summarize that

- our complexified square well generates the infinite set of real energies;
- the roots T_n which define these energies are almost equidistant, especially at the higher n;
- as expected, the standard square-well-type behaviour of the spectrum is reproduced at the small Z and for the highly excited states.

In the strongly non-Hermitian domain, the lowest doublets of states subsequently disappear. Presumably, their energies dissolve in conjugate pairs in complex plane. The $\mathcal{PT}$ symmetry of their wave functions breaks down. The related solutions become "unphysical" and have to be omitted in a way paralleling the similar "disappearance of states" at $\delta < 0$ in the model (3) of ref. [5]. The resulting sudden upward jump of the ground-state energy definitely enters the list of paradoxes, emerging in the other exactly solvable models. Their present list already involves the unavoided level crossings in the harmonic and Coulomb oscillators [15, 17], the anomalously large excitations in the $\mathcal{PT}$ symmetrized but bounded Rosen-Morse field [16], some unexpected manifestations of the strong singularities in the Pösch-Teller and Eckart models [18], and a spontaneous re-ordering of levels in the Morse asymmetric well [19].

In this context, the role of the complexified square well is as exceptional as in the Hermitian limit. We may expect that its generalizations with more points of discontinuity will remain tractable analytically. This could be of a significant help, say, within perturbation theory [23]. In the more pragmatic numerical setting, one should recollect that the so called Prüfer transformation [24] (i.e., nothing but a square-well-inspired use of the *locally* exponential solutions) found a firm place in the standard computer software [25]. Last but not least, one has to keep in mind that in the Hermitian quantum mechanics the use of the locally constant forces could also clarify the various manifestations of the pertaining Sturm Liouville theory [26]. An appropriate $\mathcal{PT}$ symmetrization of this theory is expected to be quite a difficult task [27]. In such a direction, also the knowledge of our present solutions could mediate a further progress, hopefully, in the near future.

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